

عنوان مقاله:

Quantum chemical studies on corrosion of iron in acidic and basic environments

محل انتشار:

اولین همایش ملی تکنولوژی های نوین در شیمی و پتروشیمی (سال: 1393)

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خلاصه مقاله:

In this research the corrosion behavior of iron in HCl and NaOH media were investigated. In this regard, the quantum chemical calculation was performed. Furthermore the natural bond orbital for the direction and magnitude of charge transfer interactions was calculated. The results show that the total charge transfer from hydroxide anion to the iron surface is more than from ones for chloride anion, then the corrosion of iron in NaOH solution is less than HCl solution. To verify these predictions, using Tafel plots, we studied the phenomena from experimental viewpoint. The studies confirmed that the rate of corrosion in HCl solution is substantially greater than in NaOH media

کلمات کلیدی:

iron corrosion, natural bond orbital, cluster model

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